



Benchmarking linac codes for the HIPPI Project

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INTRODUCTION

One of the main tasks of the beam dynamics working package of the European network “High Intensity Pulsed Proton Injector” (HIPPI) is the comparison and validation of 3D linac codes in the high current regime. Several codes are available and currently run for such simulations. Different approaches used to describe the space charge effects and different lattice modeling (especially regarding the RF) may pose severe problems understanding the source of discrepancies when tracking simulations at high current are run. For this reason the code benchmarking has been divided in three steps.

The first is a “static” comparison of space charge calculations: common Gaussian ensembles of particles are given as input to the codes and the Poisson solvers are run without any tracking. The resulting space charge electric fields are compared with the analytical solution against different numerical parameters and boundary conditions. To investigate the effects of numerical errors on the single particle dynamics the instantaneous depressed tune is inferred using the previous calculated space charge electric fields and compared again with an analytical solution. Both tests require modification in the source codes (that usually do not print out the space charge electric field) and have been performed on codes with source code available.

The second step consists of tracking simulation with a zero-current beam using a common Gaussian input distribution and the lattice of the UNILAC DTL section for comparison among codes. The scope of this test is dual: first the preparation of the input files for all the codes checking carefully that they describe the same structure;

second the understanding of discrepancies arising from the different representation of physical elements implemented in the codes, especially for the RF.

In the last step tracking simulations will be run in the same conditions of the experiments planned for the end of 2005: measured beam current, profiles and emittances at the DTL entrance will be used to create input distributions that best fit these values and the results will be compared with profiles and emittances measured downstream at the DTL exit.

In this paper the results of the first two tests are presented and commented. Five codes have been used so far: IMPACT [1], DYNAMION [2], TOUTATIS [3], PARMILA [4] and HALODYN [5]. Other codes, already available like PARMELA and PATH as well as codes under development at the IAP in Frankfurt and at the FZJ in Jülich, will be included in the near future. Details about the program and the benchmarking can be found in [6].

STATIC COMPARISON

In order to investigate the quality of the space charge routines of different codes we ran several tests without any tracking (to avoid “coupling” with different lattice modeling) and modified the source code to output the electric field at the position of each particle and on the grid points of the mesh box (for PIC codes only). In order to compare the results as function of numerical parameters, such as number of (macro)particles N_p and mesh resolution Δx , we abolished any box resize and adaptive remesh in the PIC codes IMPACT and TOUTATIS respectively. Since this test is not involving any tracking and the solvers are called only once, no study on the CPU time has been carried out.

Space charge electric field test

We generated three Gaussian distributions of 10^4 , 10^5 and 5×10^5 particles having $\sigma_x = \sigma_y = 4$ mm and $\sigma_z = 8$ mm and representing a 1mA $^{238}\text{U}^{+28}$ bunched beam at the energy of 1.4 MeV/u, which is the beam that will be mostly used during the measurement campaign at the UNILAC in 2005. The grid box of the PIC codes (IMPACT, TOUTATIS and HALODYN) is fixed to $L_x = L_y = 6.4$ cm and $L_z = 18.4$ cm, whereas for DYNAMION no grid must be introduced, as this code has a direct particle-particle solver. The electric field at the particle position obtained in output from the codes is compared with a semi-analytical solution obtained with an algorithm described in [7]. The error we used as figure of merit is defined as follows: only a longitudinal slice of $2\sigma_z$ is taken into account; for each particle within a cylindrical shell $r \pm \delta r$, the error is defined as follows

$$\varepsilon(r, n) = \frac{\|(E_{x_n}^C - E_{x_n}^A, E_{y_n}^C - E_{y_n}^A)\|}{\|(E_{x_n}^A, E_{y_n}^A)\|}, \quad (1)$$

and averaged over the particles in the shell, providing

$$\varepsilon(r)_{rms} = \langle \varepsilon(r, n) \rangle_{\sqrt{x_n^2 + y_n^2} \in r \pm \delta r} \equiv \frac{\delta E}{E}(r). \quad (2)$$

$(E_{x_n}^C, E_{y_n}^C)$ is the transverse electric field at the position of the n^{th} particle as computed by the code, whereas $(E_{x_n}^A, E_{y_n}^A)$ is the corresponding semi-analytical solution. Figure 1 shows the results for DYNAMION and the PIC codes with a grid resolution of 128^3 (or 129^3 according to the algorithm). Comparisons for a 64^3 (65^3) grid have been performed but not shown here. The relative error shows for all codes an exponential drop within the bunch core, whereas outside some differences appear: while the IMPACT (open boundary conditions) error keeps converging to zero, it remains on the $\sim 1\%$ level for DYNAMION, TOUTATIS and IMPACT (closed boundary conditions) and it increases up to 10% in HALODYN. Simulations with larger boundaries revealed a general improvement of this error: with a box of $L_x = 9$ cm it remains at $\sim 1\%$ level. We interpret the 100% error at the bunch center for all the codes as follows: with the electric field E going linearly to zero as $r \rightarrow 0$, the same is true for the error δE .

Single particle tune test

Even if the quality of the space charge electric field is a clear figure of merit of a solver, its error does not provide an estimation of the induced error in the beam dynamics. Resonant halo and resonance trapping and de-trapping are both mechanisms of interest in high intensity regimes. A correct description of these phenomena passes through the correct representation of the single particle dynamics, which in turn is characterized by the single particle tune (SPT) and the crossing of a resonance condition. Space charge depresses the tune due to its intrinsic defocusing characteristics. Given an ideal lattice description, i.e. a correct tune diagram, an error in

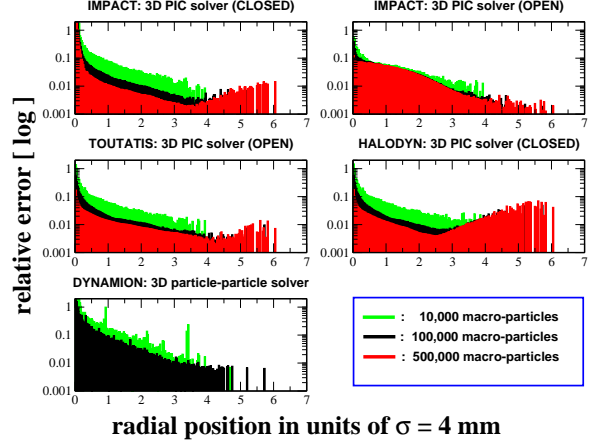


FIGURE 1. (Color) Field error defined in Eq.(2) for DYNAMION and PIC codes with a grid resolution of 128^3 (129^3).

the electric field computation results in wrong depressed SPT and inaccurate resonance crossing description.

In order to establish a common SPT test for the codes we set up the following procedure. A single test particle is made to oscillate along x (i.e. all the other coordinates and momenta are set to zero) in a constant focusing channel with a given bare tune q_0 using a simple single particle tracking routine. Superimposing the frozen space charge field, i.e. an electric field which does not change due to the internal motion of the particle distribution, the test particle will explore the entire space charge field. Recording its oscillations, the depressed SPT is inferred via FFT. For the space charge electric field originated by a Gaussian distribution, analytical formulae are available to derive the correct depressed SPT, to be compared with the one experienced by the test particle. Since the electric field computed by the code is frozen, we speak of an “instantaneous” SPT. To enhance the space charge effects, we set the bunch charge to provide a maximum tune depression of 0.7 (see Fig. 2).

This test so far has been performed for PIC codes only. To apply the space charge force to the test particle we indeed need the electric field on the grid points and an interpolation routine to infer the field at the particle position. To take into account differences in the interpolating routines of each code, the latter ones have been “exported” in the single particle tracking routine and used consistently with the code under investigation. This procedure is incompatible with the nature of a particle-particle solver like the one in DYNAMION, which has been kept out of this test.

Errors in PIC solvers are generally driven by two main factors: number of particles N_p , because of the statistical fluctuation of the number of particles within a grid cell, and grid resolution Δx . These errors drive in turn an error

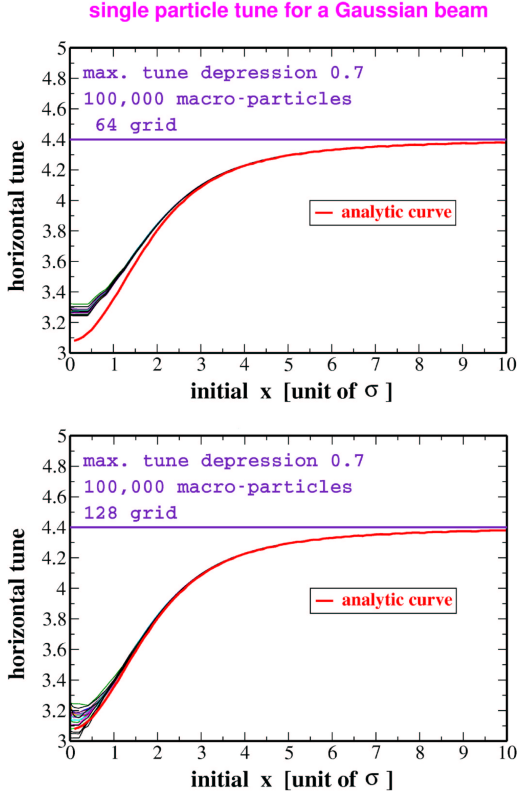


FIGURE 2. (Color) Depressed SPT from PIC simulations (IMPACT) running several 6D-Gaussian ensembles for two grid resolutions to be compared with the analytical curve.

in the depressed SPT

$$q^C = q^A + \delta q, \quad \delta q = \delta q(N_p, \Delta x),$$

where q^C and q^A are the depressed SPT from the PIC code and the analytic solution respectively, δq is the numerical error we are going to investigate. The nature of this error is both statistical and *geometrical* (limited spatial resolution). We propose a scaling law for δq at the bunch center that distinguishes the two sources

$$\delta q = K_1 \left(\frac{K_2(f_n, Vol_b)}{\sqrt{\Delta x^3 N_p}} + K_3(Vol_G, Vol_b) \Delta x^\alpha \right), \quad (3)$$

where K_1 depends on the constant focusing channel only, K_2 depends on the statistics and the bunch volume Vol_b and K_3 on both Vol_b and the grid box volume Vol_G . The power α will be inferred via data fitting. Fixing both numerical parameters and the constant focusing channel, the PIC solvers can be compared looking at the coefficients of this law: the smaller they are, the better is the solver. The choice of looking only at the bunch center will be motivated at the end of the section.

The first term in the r.s.h. $\propto (\Delta x^3 N_p)^{-1/2}$ depends basically on the number of particles per cell and introduces

a numerical “tune spread” simulating several initial particle distributions. The second one $\propto \Delta x^\alpha$ is driven by a combined effect of discretization errors in the solver and statistics and introduces a numerical “tune shift”. In Fig. 2 PIC simulations have been run using 10^5 particles and two different grid resolutions (64^3 and 128^3). The corresponding depressed SPTs are plotted together with the analytical curve. The numerical “tune shift” is clearly visible at the bunch center in the upper plot corresponding to the 64^3 grid, where there is a non-zero bias between q^C and q^A . This bias is reduced increasing the grid resolution, i.e. reducing Δx (bottom plot). The numerical “tune spread” is more visible in the 128^3 grid case (bottom plot) where q^C among the 20 simulations varies by 0.1. Simulations with 64^3 grid (upper plot) and the same number of particles show a lower “spread” due to high number of particles per cell.

The constants K_1 , K_2 and α have been inferred running *static* simulations using three sets of 20 random axisymmetric Gaussian distributions (10^5 , $4 \cdot 10^5$ and 10^6 particles) with the same RMS sizes ($\sigma_x = \sigma_y = 4$ mm and $\sigma_z = 8$ mm) and varying the grid resolution from 32^3 to 128^3 . For each code and grid resolution, the SPT

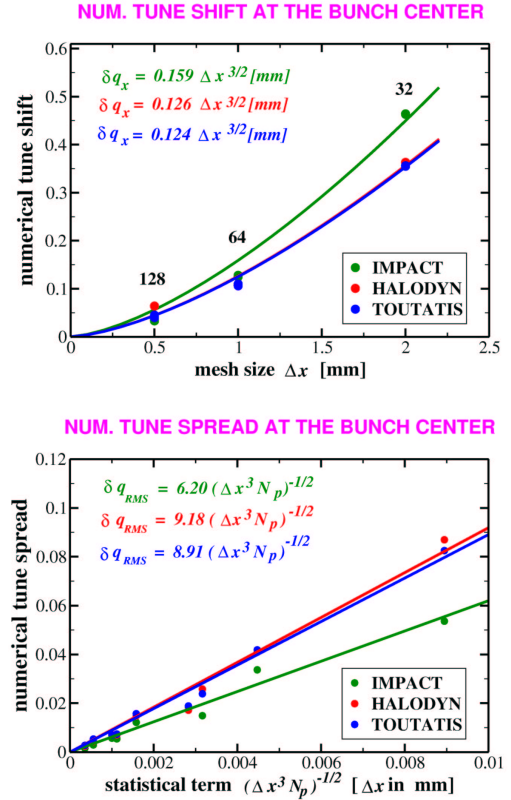


FIGURE 3. (Color) Numerical tune “spread” and “shift” and corresponding constant K_2 , K_3 and α defined in eq. (3). The fits provide χ^2 values varying from 10^{-3} to 10^{-4} .

at the bunch center has been averaged (providing the numerical “tune shift” Δq^N after subtracting the analytical value q^A) and its standard deviation (the “tune spread” $\langle \delta q \rangle$) calculated. In Fig. 3 these two quantities at the bunch center are shown together with the constants in the scaling law obtained from the fitting. Notice that in the numerical “tune shift” (upper) plot, even if only one point is visible for each grid, there are three, corresponding to the three sets of ensembles. This confirms that this term is independent on N_p . In Fig. 4 their behavior as function of the oscillation amplitude is shown. To take into account the variation of the space charge effects moving outward the bunch center, both Δq^N and $\langle \delta q \rangle$ have been normalized to the real local tune shift. The values at the bunch center are upper bound limits: over the entire bunch $\overline{\Delta q^N}$ decreases by a factor 2, whereas $\langle \overline{\delta q} \rangle$ drops by one order of magnitude.

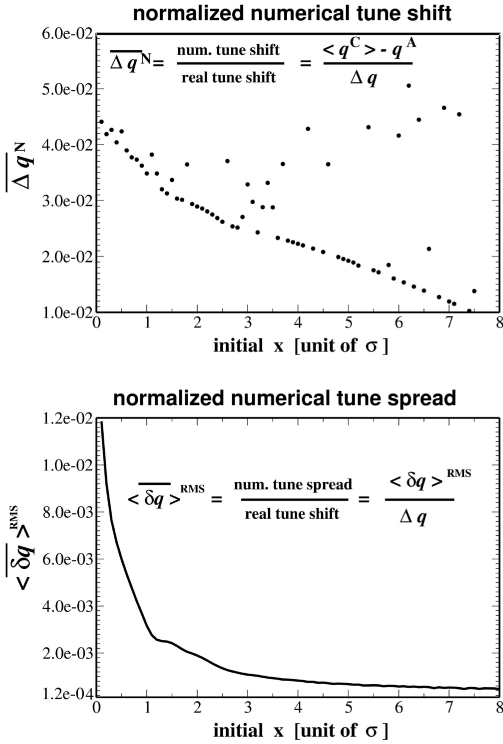


FIGURE 4. Normalized numerical “tune shift” and “tune spread” against amplitude oscillations (IMPACT).

UNILAC TRACKING AT I=0

Preliminary tracking simulations of the UNILAC DTL sections have been run using a (not matched) spherical 6D-Gaussian bunch of $\sigma_r = 2$ mm, $\sigma_p = 2$ mrad and 10^3 particles. The beam current is set to 0 to investigate the outcome of different lattice and RF modeling. SUPERFISH has been used to generate the TTF table for PARMILA and the RF (linear) maps for IMPACT. DYNAMION models the RF solving the Laplace equa-

tion in the gap region between two drift tubes, whereas HALODYN applies a thin kick at the gap center. Since TOUTATIS is an RFQ code and its extension to a generic linac structure still under development, it was kept out of this comparison. The transverse sizes and emittances (not shown here) agree within 1%, while larger differences appear in the longitudinal emittance (Fig. 5): IMPACT does not show any growth (because of the linear map), which is of about 10% in the third tank for both HALODYN and PARMILA and reaches the 40% in DYNAMION. We plan to run in the future also IMPACT simulations using the Lorentz integrator instead of the linear transfer map.

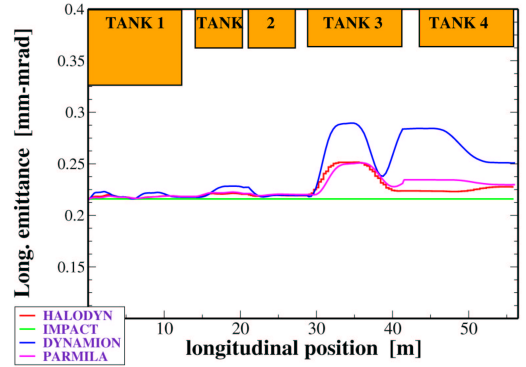


FIGURE 5. (Color) Longitudinal emittance profile at I=0.

OUTLOOK

The static comparison has shown a quite similar behavior of different space charge solvers. Tracking simulations of the DTL UNILAC section revealed larger differences in the longitudinal dynamics due to the different RF modeling. One of the next steps in the benchmarking program is to investigate how these two aspects couple in realistic tracking simulations with high current.

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